EFFECTIVE FREQUENCY TECHNIQUE

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Abstract

An effective monochromatic frequency technique is described to represent the effects of finite spectral bandwidth for active and passive measurements centered on an absorption line, a trough region, or a slowly varying spectral feature. For Gaussian and rectangular laser line shapes, the effective frequency is shown to have a simple form which depends only on the instrumental line shape and bandwidth and not on the absorption line profile. The technique yields accuracies better than 0.1% for bandwidths less than 0.2 times the atmospheric line width.

I. Introduction

The effects of finite bandwidth distort a spectral measurement by broadening the line and decreasing the apparent absorption at line center. This can produce large errors in the measured spectrum.[1] For laboratory measurements, deconvolution techniques may be used to recover the true spectrum.[2] The analysis of range resolved lidar measurements of differential absorption in the atmosphere is more complex since the spectral line shape changes with altitude and the intervening atmosphere affects the measured differential absorption at the end point of the measurement.[3,4] A method of solving for the differential absorption has been briefly discussed using a complex iteration procedure.[3,5]

In this paper, we describe a fundamentally new approach to analyze the problem of radiative transfer and atmospheric transmission with finite spectral bandwidth. We show that an equivalent monochromatic frequency may be used to represent the effects of finite bandwidth. In the vicinity of line center, the equivalent frequency can be expressed by a simple analytical form that depends on the characteristics of the instrumental distortion function rather than the nature of the spectral line profile and the particular characteristics of the path being used. The technique is applicable to radiative transfer calculations as well as to a large class of active and passive spectroscopic experiments, in both the laboratory and the atmosphere. An equivalent frequency not only greatly simplifies the computation of finite bandwidth effects for forward problems in radiative transfer but also allows the inverse problem of the remote measurement of species concentration or atmospheric properties to be solved using simplified monochromatic methods.

An integrated form of the mean value theorem provides the theoretical basis for this technique[6]. It can be shown for a finite bandwidth measurement that an equivalent frequency exists at some point within the instrumental bandwidth if the instrumental line profile is a continuous function and does not change sign. The location of the equivalent frequency is not defined, however. In this paper, we present general methods for calculating the equivalent frequency and show that the results are applicable to the whole range of spectroscopic and atmospheric line profiles.

II. Theory

For the case of finite bandwidth, the two way transmission of the atmosphere is related to the absorption coefficient $K(\upsilon,x)$, the absorption per unit path as[3]

$$\bar{\tau}_{\upsilon}(0,R)=\int_{-\infty}^{\infty}h(\upsilon)\exp\left[-2\int_{0}^{R}K(\upsilon,x)dx\right]d\upsilon \qquad (1)$$

where the integral of the instrumental line shape $h(\upsilon)$ is normalized to have unit value. In the vicinity of an absorption line centered at υ_o, the absorption coefficient may be expanded as

$$K(\upsilon,x)=a_1(x)-a_2(x)\,(\upsilon-\upsilon_o)^2+o\,((\upsilon-\upsilon_o)^4) \qquad (2)$$

where we explicitly allow for a dependence of the absorption coefficient on distance as, for example, would be encountered in the atmosphere. The quadratic expression of Eq. (2) is valid in general since a Taylor series expansion of any function about a maximum or minimum yields an equation of this functional form whereas $dK/d\upsilon|\,\upsilon_o=0$ and the linear term in the expansion is zero. Eq. (2) provides a good approximation to the absorption coefficient for bandwidths which are small compared to the absorption line width. For a collision-broadened or Doppler profile, Eq. (2) gives the absorption coefficient to accuracies better than 1% for distances up to 0.3 half-widths from the line center. Since Eq. (2) is general, it can be used to represent the absorption coefficient near line center for the Voigt line profile or even for a complex line shape such as would result by integrating Voigt profiles over an atmospheric path with varying pressure and temperature. Eq. (2) can also be used to represent the absorption in trough regions, the region of minimum absorption between two absorption lines. [7]

To evaluate the transmission for a measurement centered on an absorption line, an explicit form for the observational line shape is required. We consider first the case of a Gaussian profile, e.g.,

$$h(\upsilon)=\frac{2}{\Delta\upsilon}\left(\frac{\ln 2}{\pi}\right)^{1/2} \exp\left(-\ln 2[(\upsilon-\upsilon_o)/\Delta\upsilon/2]^2\right) \tag{3}$$

It follows from Eqs. (1), (2), and (3) that the transmission is given as

$$\bar{\tau}_\upsilon(0,R)=\left(\frac{b}{\pi}\right)^{1/2} \exp\left(-2\int_0^R a_1(x)\,dx\right)\int_{-\infty}^{\infty}\exp\{-(\upsilon-\upsilon_o)^2\,[b-2\int_0^R a_2(x)dx]\}d\upsilon \tag{4}$$

where $b=4\ln 2/\Delta\upsilon^2$. Eq. (4) can be integrated and for

$$2\int_0^R a_2(x)dx/b \ll 1, \tag{5}$$

the result can be expressed as

$$\bar{\tau}_\upsilon(0,R)=\exp\{-2\int_0^R [\,a_1(x)-a_2(x)/(2b)(1+\int_0^R a_2(x)dx/b)]dx\} \tag{6}$$

Eq. (5) is equivalent to the condition that the change in the optical depth between the center and half-width point of the measurement bandpass is small with respect to ln2. It then follows from Eqs. (1) and (2) that Eq. (6) is equivalent to

$$\overline{\tau}_\upsilon(0,R)=\exp(-2\int_0^R K\,(\,\overline{\upsilon}_e,\,x)dx),$$

where $$\overline{\upsilon}_e=\upsilon_0 \pm \Delta\upsilon/(2\sqrt{2\ln 2})(\,1+\frac{\Delta\upsilon^2}{8\ln 2}\int_0^R a_2(x)dx) \qquad (7)$$

Thus, the transmission for a measurement centered on an atmospheric line or in a trough region can be represented by an equivalent monochromatic measurement at the frequency $\overline{\upsilon}_e$ for bandwidths which are small compared to the atmospheric line width. We note that the first term for the equivalent frequency depends only on the characteristics of the instrumental distortion function.

An effective frequency can also be used to analyze finite bandwidth measurements for a measurement with a rectangular line shape. For this case, the line shape is

$$\begin{aligned} h(\upsilon)&=1/\Delta\upsilon & &|\upsilon-\upsilon_0|\leq\Delta\upsilon/2 \\ &=0 & &|\upsilon-\upsilon_0|>\Delta\upsilon/2 \end{aligned} \qquad (8)$$

and $\overline{\tau}_\upsilon(0,R)=(1/\Delta\upsilon)\int_{-\Delta\upsilon/2}^{\Delta\upsilon/2}\exp[-2\int_0^R(a_1(x)-a_2(x)(\upsilon-\upsilon_0)^2)dx]d\upsilon$

We note that a rectangular line shape provides a first order approximation to the average spectral output of a multimode laser with a frequency jitter of the order of the mode separation. From Eqs. (1), (2), (8) and an analysis similar to that given for Eqs. (4)-(7), it can be shown that for a rectangular line shape

$$\overline{\upsilon}_e=\upsilon_0 \pm\Delta\upsilon/(2\sqrt{3}) \qquad (9)$$

Eqs. (7) and (9) show that for a Gaussian or rectangluar instrumental line shape, the transmission over the atmospheric path from range 0 to R can be represented simply by the transmission at the effective frequency $\bar{\upsilon}_e$. We note that Eqs. (7) and (9) are valid for any atmospheric path.

We can also utilize the equivalent frequency for analysis of finite bandwidth effects at a reference frequency. Since a reference frequency is generally chosen either in the far wing of a line or on the edge of an absorption band where the absorption changes slowly with frequency, the absorption coefficient may be represented as a linear function of frequency for a moderately narrow bandwidth. That is,

$$K(\upsilon,x)=a(x) + b(x)(\upsilon-\upsilon_r). \tag{10}$$

For the case where the variation in the atmospheric optical depth is small over the line shape, i.e.,

$$2(\upsilon-\upsilon_r)\int_o^R b(x)\,dx \ll 1, \tag{11}$$

it follows that the corresponding term in the transmission in Eq. (1) can be expanded which yields

$$\bar{\tau}_r(0.R)=\exp(-2\int_o^R a(x)dx)\int_{-\infty}^{\infty} h_\upsilon[1-2(\upsilon-\upsilon_r)\int_o^R b(x)dx]d\upsilon \tag{12}$$

For a line shape which is symmetric about υ_r, h (υ) $(\upsilon-\upsilon_r)$ is an odd function (e.g., with zero integral) and Eq. (12) reduces to

$$\bar{\tau}_r\,(0,R)=\exp(-2\int_o^R K(\upsilon_r,x)dx) \tag{13}$$

and $\bar{\upsilon}_e=\upsilon_r$

Thus, the transmission in the region of the reference frequency can be represented by an equivalent monochromatic measurement at the center of the bandpass for any instrumental line shape which is symmetric providing the absorption coefficient is a linear function of frequency.

III. Application to Differential Absorption

Consider a two-frequency lidar measurement of the resonant absorption for an atmospheric species (e.g., CO_2 or H_2O) or property (e.g., temperature or pressure) where the measurement at each frequency is made with a finite bandwidth laser. The measurement at the on-line frequency υ is typically centered on an absorption line of the desired atmospheric species. A reference frequency υ_r is then selected at a nearby location where the resonant absorption is weak compared to that at the measurement frequency. The two frequencies are chosen sufficiently close, however, so that the atmospheric backscatter and the attenuation due to both scattering and continuum absorption processes is essentially identical at the two frequencies. The ratio of the signal returns backscattered from the atmosphere at two adjacent frequencies at ranges R_1 and R_2 essentially eliminates the scattering and absorption properties of the atmosphere, except for those of the resonant absorption effect to be measured. For elastic scattering and homogeneous scattering and absorption over a range gate of width ΔR, it follows from the lidar equation[8] that the ratio R of the energy at the on-line and reference frequencies from two successive range gates is given as

$$R = \frac{\bar{\tau}_\upsilon(0,R_2)/\bar{\tau}_r(0,R_2)}{\bar{\tau}_\upsilon(0,R_1)/\bar{\tau}_r(0,R_1)} \tag{14}$$

where

$$R = \frac{\varepsilon_\upsilon(R_2)/\varepsilon_r(R_2)}{\varepsilon_\upsilon(R_1)/\varepsilon_r(R_1)}$$

and where $\bar{\tau}_{\upsilon}(0,R)$ and $\bar{\tau}_{r}(0,R)$ are the transmission along the two-way path path from 0 to R for laser bandwidths centered at the on-line frequencies υ and the reference frequency υ_r, respectively, and ε (R) is the energy received from an element of the atmosphere at range R with thickness ΔR, and $R_2=R_1+\Delta R$.

The inclusion of finite laser bandwidth effects and non-zero resonant absorption at the reference frequency complicates the analysis of Eq. (14) considerably since the differential absorption coefficient, $K(\upsilon) - K(\upsilon_r)$ is not a directly measured or easily derived quantity. In addition, the differential ranging measurement given by Eq. (14) not only has absorption information in the desired range element of width ΔR centered at $R=(R_1+R_2)/2$, but also contains absorption information from the region 0 to R_1.

If an effective frequency is used to represent the absorption at the reference frequency (i.e., Eq. (13)), it follows that a differential absorption measurement with differential ranging and finite bandwidth at both the on-line reference frequencies can be represented as

$$R = \frac{\int_{-\infty}^{\infty} h(\upsilon)\exp\left\{-2\int_0^{R_2}[K(\upsilon,x)-K(\upsilon_r,x)]dx\right\}d\upsilon}{\int_{-\infty}^{\infty} h(\upsilon)\exp\left\{-2\int_0^{R_1}[K(\upsilon,x)-K(\upsilon_r,x)]dx\right\}d\upsilon} \qquad (15)$$

where $h(\upsilon)$ is the laser line shape for the on-line measurement. Eq. (15) has the form of a differential absorption experiment. We note that Eq. (15) is valid even for the case of strong absorption in the region of υ_r since no assumptions on the overall level of absorption were made.

An effective frequency can also be used to greatly simplify the analysis of finite bandwidth measurement at the on-line frequency. It follows from Eq. (15) that a differential absorption measurement with differential ranging and finite bandwidth can be expressed in terms of the effective frequencies $\bar{\upsilon}_e$ and υ_r as

$$R = \exp\{-2\int_{R1}^{R2} [\, K(\bar{\upsilon}_e,x)-K(\upsilon_r,x)]dx\}. \tag{16}$$

Thus, the effective frequency method reduces the problem of measurements with finite bandwidth at the on-line and reference measurements from a relatively untractable form, where the measured quantity is a complex function and depends on the absorption over the entire atmosphere path, to a simple measurement of the differential absorption coefficient, $K(\bar{\upsilon}_e,x) - K(\upsilon_r,x)$, over the desired measurement interval from R_1 to R_2.

IV. Comparison with Simulation

To evaluate the application of the effective frequency technique, we consider the case of generalized absorption in the atmosphere. The absorption coefficient of a gas species in the atmosphere at frequency υ is [3]

$$K(\upsilon)=qnS(T)f(\upsilon-\upsilon_o), \tag{17}$$

where q is the molecular mixing ratio of the species, n is the number density at pressure p and temperature T, S (T) is the line strength, and $f(\upsilon-\upsilon_o)$ is the line shape at frequency υ for a line centered at υ_o. For atmospheric measurements where the effects of both collision and Doppler broadening contribute significantly to the absorption, the line shape is given by the Voigt profile[9] which is a convolution of independent Lorentz and Doppler profiles. It is given as

$$f(\upsilon-\upsilon_o)=\frac{f' a}{\pi}\int_{-\infty}^{\infty}\frac{\exp(-y^2)dy}{a^2+(\zeta-y)^2}, \tag{18}$$

where

$$f'=(\ln 2/\pi)^{1/2}b_d,$$

$$a=(\ln 2)^{1/2}b_c/b_d,$$

$$\xi=(\ln 2)^{1/2}(\upsilon-\upsilon_o)/b_d \tag{19}$$

and b_c and b_d are the collision broadened and Doppler broadened line half-widths at half-height, respectively. These are defined as

$$b_c(p,T)=b_c^o(T_0)(p/p_0)(T_0/T)^m,$$

$$b_d(T)=[2kT\ln 2/(M_0\,c^2)]^{1/2}\upsilon_0, \tag{20}$$

where M_0 is the mass of the absorbing species, c is the velocity of light, p_0 is standard pressure, b_c^o (T) is the collision-broadened line half-width at a pressure of one atmosphere and the exponent of the temperature dependence of the collision-broadened half-width m is predicted to be 1/2 from kinetic theory.

To evaluate the error in the determination of the differential absorption coefficient using an effective frequency, Eq. (15) was evaluated numerically for rectangular and Gaussian laser line shapes of various widths using Eqs. (17) and (18). The atmospheric model used for evaluating Eq. (17) is a multilayer, one-dimensional model with up to 50 homogeneous layers. The calculations simulated measurements for a two-way atmospheric path from infinity to various altitudes for a total optical depth of two at line center. The altitude of the end point of the measurement is represented by the pressure at that altitude as given by the parameter "a" which is proportional to pressure. The calculations thus begin with a Doppler profile at high altitude, a=0, and include all values of “a” for the Voigt line profile up to and including the value of ‘a” at the end point of measurement.

Figures 1A and 1B give the error between this detailed evaluation of the differential absorption coefficient and the analysis using a monochromatic calculation at the effective frequency for the cases of Gaussian and rectangular laser line shapes, respectively. The errors are shown as a function of the ratio of the laser bandwidth, the full width at half height, to the half-width at half-height of the Voigt line profile at the end point of the measurement, b_υ and a. For values of $\Delta\upsilon/b_\upsilon$ less than 0.5, the error in using an effective frequency is less than 0.5% for a rectangular line shape and less than 1% for a Gaussian. Accuracy at the 0.1% level can be obtained for values of $\Delta\upsilon/b_\upsilon$ less than 0.2 for a rectangular line shape or at the 0.2% level for a Gaussian..

V. Conclusion

In conclusion, we have shown that an effective monochromatic frequency can be used to represent the effects of finite instrumental bandwidth for spectral measurements centered on an absorption line, a trough region, or a slowly varying spectral feature. The technique is applicable to both integrated path and differential ranging experiments and the resulting frequency is independent of the atmospheric line shape and path, to first order. The application of an effective frequency technique greatly simplifies the analysis for a large number of spectroscopic problems. Analyses similar to those we have presented for Gaussian and rectangular line shapes can be used to derive the effective frequency for other instrumental line shapes. Complex line shapes, including multimode structure, can also be represented by a set of effective frequencies which correspond to a superposition of elementary forms.

References

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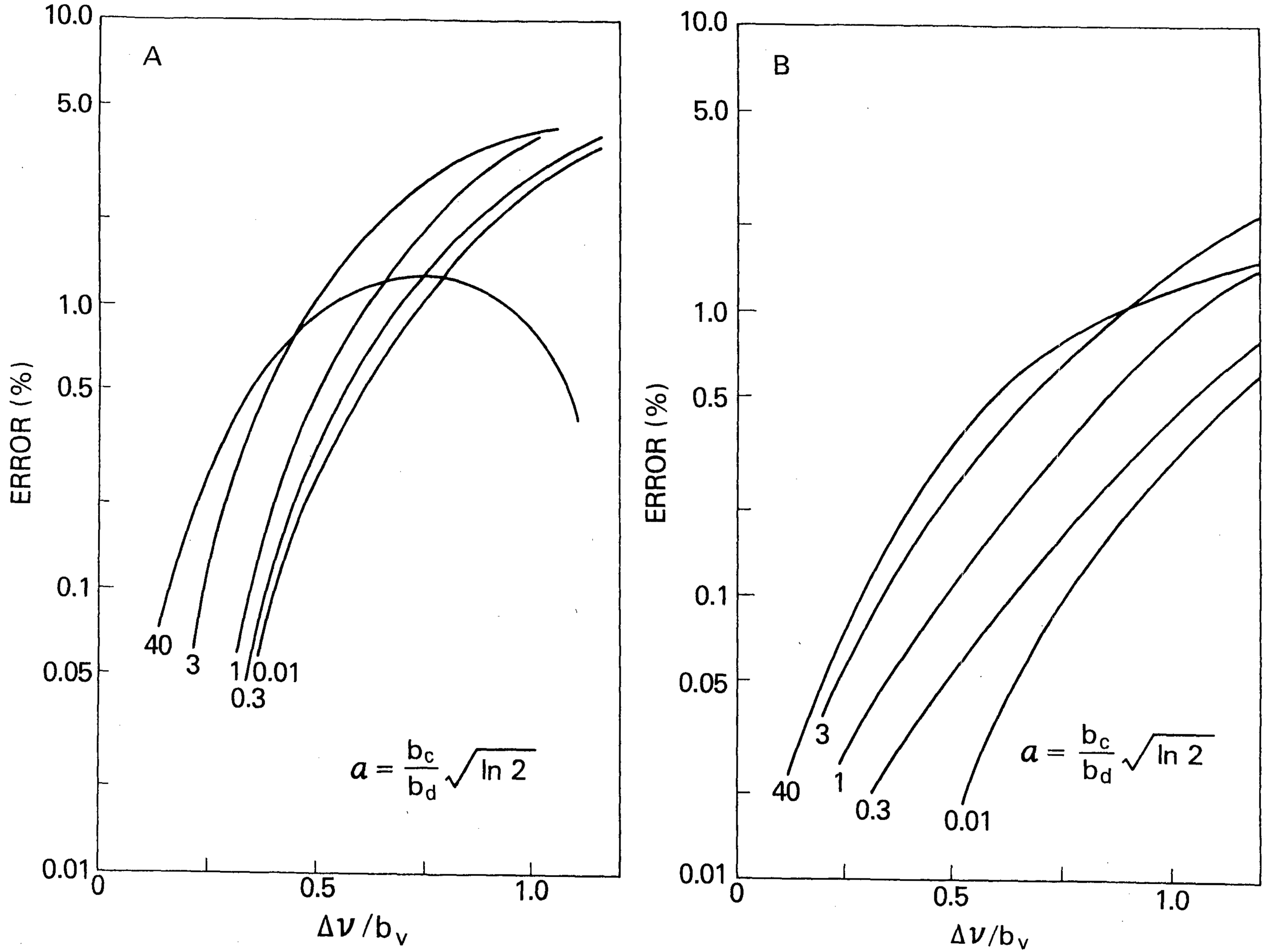
Figure Captions

Figure 1A and 1B. The percentage error in the differential absorption coefficient, as a function of the laser bandwidth to the half-width at half-height of the Voigt line profile, using a monochromatic calculation at an effective frequency to represent the effects of finite laser bandwidth. Figures 1A and 1B are for the cases of Gaussian and rectangular laser line shapes, respectively, for a downward viewing experiment from space to an altitude (pressure) in the atmosphere defined by the Voigt parameter $a=(b^{o}_{c}p/b_{d})\sqrt{\ln 2}$.


A
ERROR (%)
10.0
5.0
1.0
0.5
0.1
0.05
0.01
0
0.5
1.0
40
3
1
0.01
0.3
$a = \frac{b_c}{b_d}\sqrt{\ln 2}$
$\Delta\nu / b_v$
B
ERROR (%)
10.0
5.0
1.0
0.5
0.1
0.05
0.01
0
0.5
1.0
3
40
1
0.3
0.01
$a = \frac{b_c}{b_d}\sqrt{\ln 2}$
$\Delta\nu / b_v$

POPULAR SUMMARY

This paper describes a fundamentally new and simple approach to calculating the percent of energy transmitted over any atmospheric path or through a gas cell. These calculations are important for determining the amount of pollution in the atmosphere or for determining the amount of atmospheric heating due to 'the greenhouse effect'. Normally, calculations such as these are complex and require a computer to do thousands of computations to represent the effects of each color of the spectrum that is involved in the process. These calculations usually also depend on many other characteristics such as the particular atmospheric path, the characteristics of the absorbing gas, and the characteristics of the instrument used to do the measurement.

We have shown that rather than having to do these calculations for each color of the spectrum that is involved, we only have to do the calculations at a single effective color that represents the average effect of all the colors involved in the process. We have shown that this average effective color has a simple form that depends only on the nature of the averaging or measuring process and not on the characteristics of the atmospheric path or the absorbing gas.

This technique is applicable to a large class of calculations and measurements both in the laboratory and the atmosphere. This method allows accuracies in the calculation or measurement of the percent of energy transmitted by a gas to be as high as 99.9%. Simplifying the calculation and analysis of measurements reduces the need for thousands of computations to a single computation that a high school student could do with a good calculator.